# A Simulation Study on Kernel Density Estimation

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### What is Density Estimation?

- One of the most fundamental and important concept in statistics is the *probability density function* of a random variable X.
- ▶ In practice, when we deal with data in real life, it is too much unrealistic to think that the density *f* will be known.
- ▶ Then a natural question arises that in this kind of scenario , what to do?
- ▶ The main motive of this presentation is an attempt to answer this question.
- ▶ Let's see ☺.

#### What is Density Estimation?

- Suppose, we have a set of observed data points assumed to be a sample from a distribution with unknown pdf f .
- $\blacktriangleright$  Density Estimation is a method to construct an estimate of this unknown density f .
- One approach can be parametric density estimation i.e. we assume that the distribution from where the data is drawn, is a known parametric family and we just have to find the estimates of the parameters which characterize the distribution.
- ▶ But, the form of the density is also seldom known to us.
- Hence, we make our assumptions less rigid about the distribution of the observed data.
- ▶ This approach is **nonparametric density estimation**.
- ▶ The focus of discussion will be on this nonparametric approach.

# An Approach to Visualize - Histograms

- To get an idea about any kind of data, it is very helpful if we can visualize it properly.
- ▶ In our problem, we can serve that purpose with *Histograms*.
- ▶ Infact, histogram is the oldest and most widely used density estimator.
- Let, our origin  $= x_0$  and bin width = h, define the bins of our histogram to be the intervals  $[x_0 + mh, x_0 + (m+1)h)$ , for +ve and -ve integers m.
- ▶ The histogram is hence defined as :

$$\hat{f}(x) = \frac{1}{nh}$$
 (no of  $X_i$  in the same bin as x)

- To construct the histogram, we have to choose both origin  $x_0$  and binwidth h, but it is the binwidth h that plays the key role in the amount of smoothing.
- ▶ We will see this fact verified shortly through our simulation.

# Histograms by varying number of bins

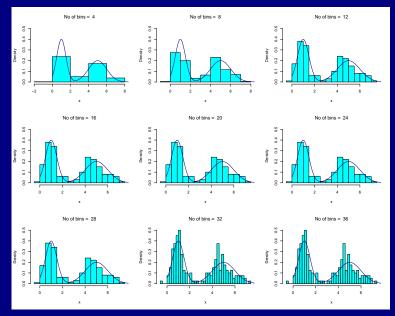
▶ A sample  $X_1, X_2, ..., X_n$  of size n = 200 from the density

$$f(x) = \phi(2(x-1)) + \frac{1}{2}\phi(x-5)$$

where  $\phi(x) = \frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}}$  is drawn.

- Then we plot the histograms of this sampled data for different number of bins.
- See all the plots for varying number of bins or equivalently varying binwidth on the same panel to catch the difference:-

# Histograms for varying number of bins



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# Observations

- ▶ If number of bins is too small (equivalently binwidth is large), the histogram is not able to estimate or *mimic* the true distribution very well , in our case , it underestimates the values of the true density at some points.
- Similarly, if we take the number of bins to be too large , then also the histogram does not perform good enough. In contrary to the previous situation, it overestimates the values of the true density at some points.
- ▶ If we take a look at the plots in the middle, they give the best estimate among all the plots available.
- Hence, our takeaway from this visualization is that neither we should decrease the binwidth arbitrarily nor should we make the bins too thick.
- Thus, one of our main challenges is to find the **best choice of** h or **optimum binwidth** h<sub>opt</sub> for our estimator.
- ▶ We will somehow try to achieve this goal through different approaches.

## **Drawbacks of Histogram**

- Subjective choice of origin.
- ▶ Bin width can be subjective.
- Discontinuity.
- Derivatives of density function cannot be estimated.
- Difficult to extend this idea to high dimensions.

### The Naive Estimator

▶ By definition,

$$f(x) = \lim_{h \to 0} \frac{1}{2h} P(x - h < X < x + h)$$

- For any given h, it is quite intuitive to estimate
   P(x − h < X < x + h) by the proportion of sample points falling in the interval (x − h, x + h).</li>
- ▶ Hence, a natural estimator is

$$\hat{f}(x) = \frac{1}{2hn} [\text{no. of } X_i \text{ falling in } (x - h, x + h)]$$

- ▶ We shall call this estimator the *Naive Estimator*.
- ►  $x h < X_i < x + h \Rightarrow -1 < \frac{x X_i}{h} < 1$
- ▶ So,to define our naive estimator more mathematically, define

$$w(x) = \frac{1}{2} I_{\{|x|<1\}}$$

▶ Then, the naive estimator is defined as:-

$$\widehat{f}(x) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{h} w\left(\frac{x - X_i}{h}\right)$$

► Due to some drawbacks hence we try to generalize this concept. \_\_\_\_\_\_

# Any Improvement??

- ▶ Takes care of the origin issue.
- ▶ All other drawbacks remain as they are.



#### Kernel Density Estimator

- We just replace the function w by a kernel function Ksatisfying  $\int_{-\infty}^{\infty} K(x) dx = 1$ .
- Usually (not always), K will be a symmetric pdf.
- Assume  $\sup_x K(x) \le M, |x|K(x) \to 0$  as  $|x| \to \infty$
- ► Assume  $K(x) = K(-x); x \in \mathbb{R}, \int_{-\infty}^{\infty} x^2 K(x) dx < \infty$
- ▶ The Kernel Type Estimator is thus given by :

$$f_n(x) = \frac{1}{nh_n} \sum_{i=1}^n K(\frac{x - X_i}{h_n})$$

 $h_n \to 0 \text{ as } n \to \infty$ 

# **Demonstrating how KDE Works**

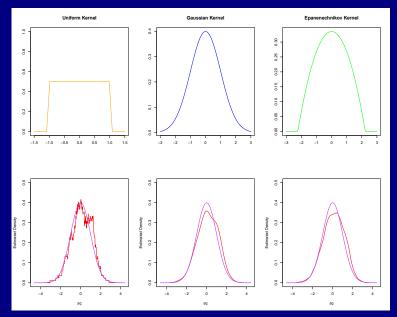
Estimated Density Function 0.4 0.3 Density 0.2 0.1 0.0 -2 -3 -1 2 3 Observed Samples

# Some examples of Kernel Functions

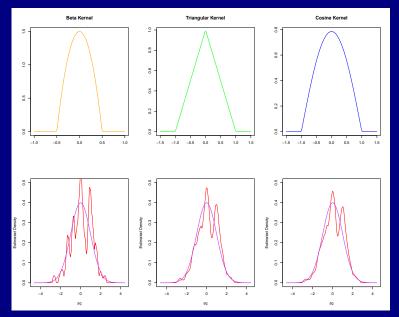
Kernel Names	$\begin{array}{c} \text{Functional Form} \\ (K\left(x\right)) \end{array}$	Efficiency relative to Epanechnikov Kernel
Uniform	$rac{1}{2}oldsymbol{I}_{ x \leq 1}$	92.9%
Triangular	$\left(1- x  ight)oldsymbol{I}_{ x \leq 1}$	98.5%
Epanechnikov	$rac{3}{4\sqrt{5}}\left(1-rac{t^2}{5} ight)oldsymbol{I}_{ x \leq\sqrt{5}}$	1
Gaussian	$rac{1}{\sqrt{2\pi}}e^{-rac{t^2}{2}}oldsymbol{I}_{x\in\mathbb{R}}$	95.1%
Cosine	$\frac{\pi}{4}\cos\left(\frac{\pi}{2}x\right)\boldsymbol{I}_{ x \leq 1}$	99.9%

Here, we have done a comparative study between these kernels to show our results. To compare how different choices of kernels influence the estimated density, we make the KDE plots for the same observed data and different kernels.

# Comparison between different kernels



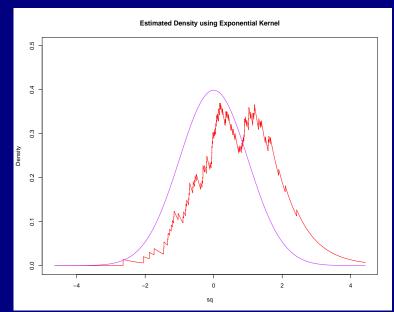
# Comparison between different kernels



#### Asymmetric kernels-how they behave?

- Though it's usually assumed in KDE literature that the kernel function K(x) is symmetric, it's of no harm to observe what happens if we take K(x) to be asymmetric also.
- For e.g we can choose our kernel as  $K(x) = e^{-x} I_{x \ge 0}$
- ▶ Let's take a look at the plot of the estimated density.

### Asymmetric kernels-how they behave?



### Observation

- In the previous diagram, we have compared our estimated density to the true density.
- ▶ We have a very very interesting observation to make here.
- The estimated kernel underestimates the true density for smaller values of x and for larger values of x, it overestimates the density.
- ▶ Why does this happen?

### Observation

The reason behind this is the form of the kernel density estimate at any point x is defined as

$$\widehat{f}_n(x) = \frac{1}{nh} \sum_{i=1}^n K\left(\frac{x - X_i}{h}\right)$$
$$= \frac{1}{nh} \sum_{i=1}^n e^{-\frac{x - X_i}{h}} I_{\left\{\frac{x - X_i}{h} \ge 0\right\}}$$
$$= \frac{1}{nh} \sum_{i=1}^n e^{-\frac{x - X_i}{h}} I_{\left\{x \ge X_i\right\}}$$

- Note that, the estimated value at x depends on only the observations that lie on the left of x.
- If we move from left to right in the plot, number of  $X'_is$  increase.
- ▶ As a consequence they contribute more and more to the estimated value.
- On the left portion, lesser number of points contribute which results in such a type of estimated density.

# Kernel-Smoothed Cumulative Distribution Function

Since, we define the kernel density estimator as :-

$$\widehat{f}_{n}(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - X_{i}}{h}\right)$$

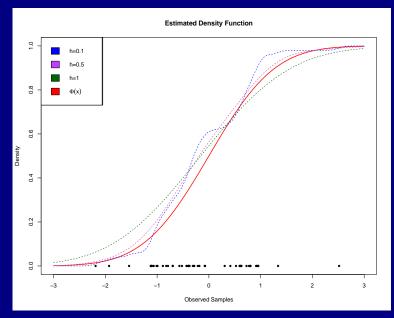
where K(.) is the kernel function, an obvious extension of this idea is to make smoothed estimators of CDF as :-

$$\widetilde{\widehat{f}}_{n}(x) = \int_{-\infty}^{x} \widehat{f}_{n}(t) dt$$
$$= \int_{-\infty}^{x} \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{t-X_{i}}{h}\right) dt$$
$$= \frac{1}{n} \sum_{i=1-\infty}^{n} \int_{-\infty}^{x} \frac{1}{h} K\left(\frac{t-X_{i}}{h}\right) dt$$
$$= \frac{1}{n} \sum_{i=1}^{n} \widetilde{K}\left(\frac{x-X_{i}}{h}\right) dt$$

#### Kernel Smoothed CDF Estimators

- where  $\widetilde{K}(x) = \int_{-\infty}^{x} K(t) dt$  is the cumulative function formed using the kernel function.
- We plot the kernel smoothed estimate CDF for a sample from standard normal distribution for different choices of smoothing parameter *h*.
- We also plot the population CDF for standard normal distribution with this.
- ▶ Let's take a look at the plot for different choices of bandwidths.

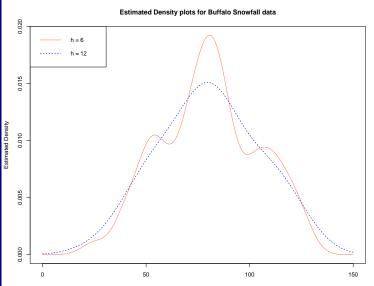
### Kernel Smoothed CDF Estimators



# **Subjective Choice**

- A natural method for choosing the smoothing parameter is to plot out several curves and choose the estimate that is most in accordance with one's prior ideas about the density.
- For many applications this approach will be perfectly satisfactory. Indeed, the process of examining several plots of the data, all smoothed by different amounts, may well give more insight into the data than merely considering a single automatically produced curve.
- Consider, as an example, the estimate given in following plot, the data underlying these estimates are the amounts of winter snowfall (in inches) at Buffalo, New York, for each of the 63 winters from 1910/11 to 1972/73.

### Kernel estimates for annual snowfall data



#### Observation

- It can be seen from the plot that varying the smoothing parameter yields essentially two possible explanations of the data, either a roughly normal distribution or a trimodal curve suggesting a mixture of three populations approximately in the ratio 1:3:1.
- For many purposes, particularly for model and hypothesis generation, it is by no means unhelpful for the statistician to supply the scientist with a range of possible presentations of the data. A choice between the two alternative models suggested by our figures is a very useful step forward from the enormous number of possible explanations that could conceivably be considered.

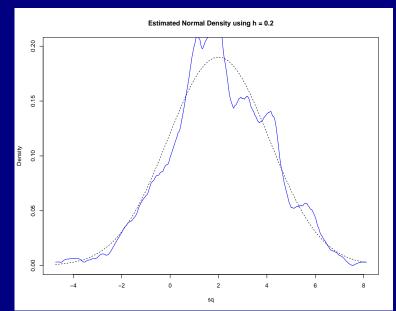
#### Reference to a standard distribution

If we assume a standard family of distributions while estimating the density, then we can obtain an exact expression of the optimal bin width  $h_{opt}$ . For example if we assume the density to be normally distributed with variance  $\sigma^2$ , and if we use gaussian kernel for estimation (i.e.  $K(x) = \phi(x)$ ), then we get :-

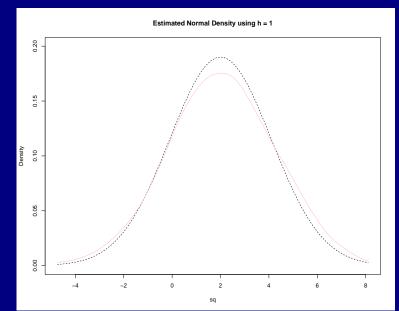
$$h_{\text{opt}} = (4\pi)^{-1/10} \left(\frac{3}{8}\pi^{-1/2}\right)^{-1/5} \sigma n^{-1/5}$$
$$= \left(\frac{4}{3}\right)^{1/5} \sigma n^{-1/5} = 1.06\sigma n^{-1/5}$$

We draw a sample of size n = 500 from a  $N(0, \sigma^2 = 4.41)$  distribution which gives  $h_{\text{opt}} \approx 0.628$ .

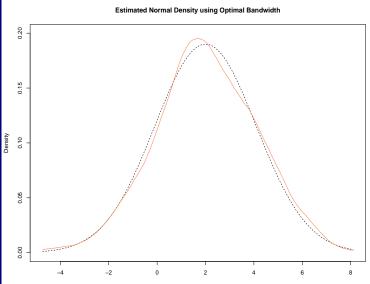
# Effect of Undersmoothing



# **Effect of Oversmoothing**



# Using optimal bandwidth



- Assume  $X_1, X_2, ..., X_n$  are iid random variable having unknown density f.
- Let  $\widehat{f}(x)$  is any estimator of the density f(x).
- The integrated squared error of  $\widehat{f}(x)$  is

$$\int (\hat{f}(x) - f(x))^2 dx = \int (\hat{f}(x))^2 dx - 2 \int \hat{f}(x) f(x) dx + \int (f(x))^2 dx$$

• The last term doesn't depend on  $\hat{f}(x)$  so we want to minimize,

$$R(\hat{f}) = \int (\hat{f}(x))^2 dx - 2 \int \hat{f}(x) f(x) dx$$

• The basic principle of least square cross validation is to construct a estimator of  $R(\hat{f})$  and minimise the estimator with respect to h.

•  $M_0(h)$  is an estimator of  $R(\hat{f})$ , Which is defined as

$$M_o(h) = \int f(x)^2 dx - \frac{2}{n} \Sigma \hat{f}_{-i}(X_i)$$

Since we can think of the histogram as an estimator of the density function as :-

$$\widehat{f}_n(x) = \frac{1}{nh}$$
 (no of  $X_i$  in the same bin as  $x$ )

- we can also find an approximate value of the optimal binwidth for histogram using cross validation method.
- ▶ Since, the cross-validation estimator of risk is :-

$$M_{0}(h) = \int \widehat{f}_{n}^{2}(x) \, dx - \frac{2}{n} \sum_{i=1}^{n} \widehat{f}_{-i}(X_{i})$$

• We will find our optimum value of h by minimising this quantity.

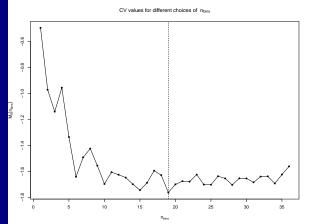
 We demonstrate the fact using a simulation study where we use our old sample of size 200 from the density

$$f(x) = \phi(2(x-1)) + \frac{1}{2}\phi(x-5)$$

• where  $\phi(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$  is the standard normal density.

- Without loss of generality, we transform this observations linearly so that they lie in the range [0,1] by doing the transformation  $y_i = \frac{x_i \min_{1 \le j \le n} (x_j)}{\max_{1 \le j \le n} (x_j) \min_{1 \le j \le n} (x_j)}.$
- We take a range of values of  $n_{bins}$  as  $\{1, \ldots, 40\}$  and then, for each of the choices we calculate  $M_0(h)$  where  $h = \frac{1}{n_{bins}}$  is the binwidth since we have normalized the range to [0, 1]. (Hence,  $n_{bins}h = 1$ .)

► After calculating the risk estimates, we plot them and the plot looks like this :-



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▶ So from the plot we can see that the estimated risk is minimum when  $n_{bins} = 19 \implies h \approx 0.0526$  and indeed it is quite similar to the heuristic observations, we made earlier.

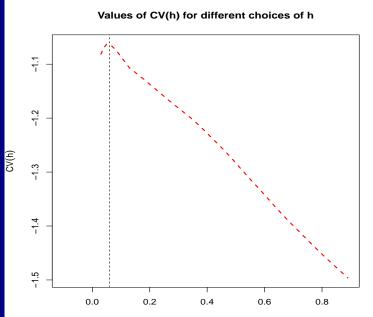
### Likelihood Cross-validation

- $X_1, X_2, ..., X_n$  are iid observations with density  $f. \hat{f}_n$  is a kernel density estimator of f with using kernel K.
- Suppose we have an observation Y from density f. Then the log likelihood of f is log f(Y).
- $\hat{f}_n$  is a parametric family of densities depending on h.
- The log likelihood of h is  $log \hat{f}_n(Y)$ .
- Since Y is not available, we can omit  $i^{th}$  of the observation  $(X_i)$  from the sample and reconstruct the density estimate  $\hat{f}_{-i}$  and the use  $X_i$  as Y. This would give the log likelihood as  $log\hat{f}_{-i}(X_i)$ . We can evaluate  $log\hat{f}_{-i}(X_i)$  by omitting  $X_1, X_2, ..., X_n$  and average out.
- ▶ The score function is

$$CV(h) = n^{-1} \sum_{i} log \hat{f}_{-i}(X_i)$$

• We can find the optimal value of h by maximising CV(h).

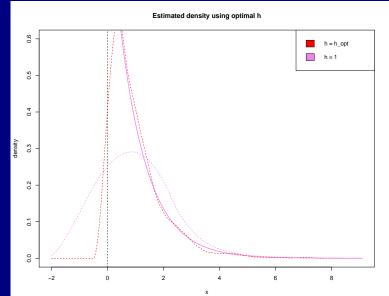
#### Likelihood Cross-validation



### Optimal Bandwidth in case of an exponential data

- In this simulation study, we first draw a random sample of size 100 from a exponential population with mean 1.
- Then we use the likelihood cross validation technique to find out the optimal value of h.
- ▶ We obtain  $h_{opt} \approx 0.06$  and then using this optimal bandwidth we plot the estimated kernel density.
- ► In order to understand the importance of choosing optimal bandwidth, we make the plots for some other choice of h like h = 1.
- Let us have a look at them.

## Optimal Bandwidth in case of an exponential data



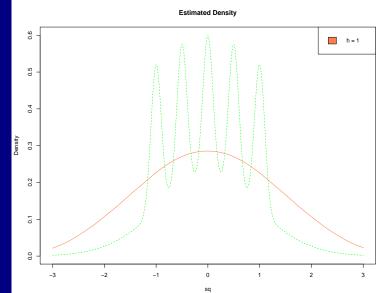
#### Observation

- We can clearly see how drastically the estimated density changes if we take choices of *h* other than the optimal one as it fails to capture the asymptotic nature of the density near 0.
- Another important drawback to mention here is that the estimated density is non-zero for negative values of x as well which is occuring due to positive weight that is being assigned due to observations whose values are near zero.

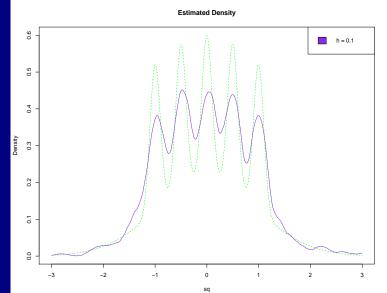
Suppose we generate a random sample of size 1000 from a density f(x) of the form :-

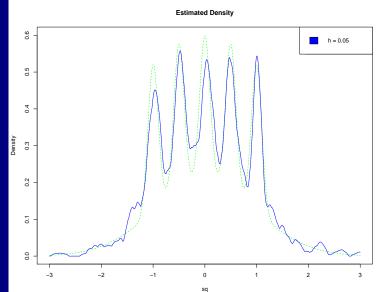
$$f(x) = \frac{1}{2}\phi(x;0,1) + \sum_{i=1}^{4}\phi\left(x;\left(\frac{i}{2}-1\right),\frac{1}{10}\right)$$

We have estimated this "claw shaped" density known as "Bart Simpson" density using **epanechnikov** kernel based on the sample observations.



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#### Observation

- ▶ For large bin width the kernel density is undersmoothed. The estimated density doesn't resemble the true density.
- For a particular value of bin width the kernel density estimates the true density precisely.
- For small bin width, the estimated kernel density is over smoothed and it doesn't capture the true nature of the density.
- ▶ So, it is very crucial to find the optimal bin width for estimating the density using kernel estimation.

#### Limiting Distribution of $V_n$

• If K(.) is a kernel function of bounded variation and the series  $\sum_{n=1}^{\infty} e^{-\gamma n h_n^2}$  converges  $\forall \gamma > 0$  where  $h_n$  denotes the bandwidth. Then

$$V_n = \sup_{x} \left| \widehat{f}_n(x) - f(x) \right| \to 0 \text{ w.p. } 1$$

- Assumption 1 For  $h_n > 0$  and  $h_n \to 0$  as  $n \to \infty$ .
- Assumption 2 K(.) is a probability probability density on R such that K(.) is right continuous, of bounded variation on R,
- ▶ and

$$\int_{-\infty}^{\infty} |u| K(u) \, du < \infty$$

• Assumption 3 K(.) satisfies the following two conditions

$$\int_{-\infty}^{\infty} uK(u) \, du = 0, \int_{-\infty}^{\infty} u^2 K(u) \, du < \infty$$

#### Convergence Rate of $V_n$

▶ Under these conditions it can be shown that<sup>58</sup>:-

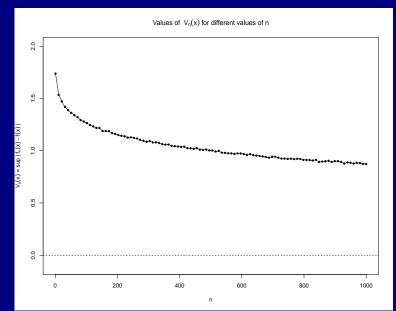
$$\sup_{x} \left| \widehat{f}_{n}(x) - f(x) \right| = O\left[ n^{-1/2} h_{n}^{-1} \left( \log \log n \right)^{1/2} \right]$$

▶ and if we choose  $h_n = n^{-1/4}$  then we have :-

$$\sup_{x} \left| \widehat{f}_{n}(x) - f(x) \right| = O\left[ n^{-1/4} \left( \log \log n \right)^{1/2} \right]$$

▶ which indicates that the rate at which  $\sup_x |\widehat{f}_n(x) - f(x)|$  goes to 0 is very slow which can also be verified from the plots we made using simulation

#### Asymptotic distribution of $V_n$



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- We assume that f is continuous at x.
- $\hat{f}_n(x)$  is the estimated density of f.

$$\hat{f}_n(x) = n^{-1} \sum_{k=1}^n Z_{nk}$$

▶ Where,

$$Z_{nk} = h_n^{-1} K[(x - X_k)/h_n]$$

▶ are i.i.d random variables. A necessary and sufficient condition for

$$\{\hat{f}_n(x) - E(\hat{f}_n(x))\} \{ var(\hat{f}_n(x)) \}^{-\frac{1}{2}} \xrightarrow{\mathcal{L}} N(0,1)$$

• is that, for every  $\varepsilon > 0$ .

$$nP[|Z_{n1} - E(Z_{n1})| \{var(Z_{n1})\}^{-\frac{1}{2}} \ge \varepsilon n^{1/2}] \longrightarrow 0 \quad as \ n \longrightarrow \infty$$

▶ A sufficient condition for

$$\frac{\hat{f}_n(x) - E(\hat{f}_n(x))}{\sqrt{var(\hat{f}_n(x))}} \xrightarrow{\mathcal{L}} N(0,1)$$

is that, for some  $\delta > 0$ 

$$\frac{E|Z_{n1} - E(Z_{n1})|^{2+\delta}}{n^{\delta/2} [var(Z_{n1})]^{1+\delta/2}} \longrightarrow 0 \ as \ \mathbf{n} \to \infty$$

which is satisfied by the Epanechnikov kernel.

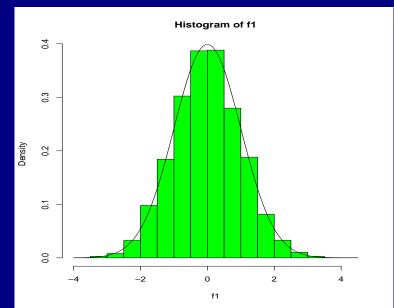
- ▶ Now, we use simulation to verify the result stated above.
- ► Suppose, we have drawn a samples from standard normal distribution. Then f(x) = φ(x) which is a continuous function.
- We have estimated the true density using the epanechnikov kernel with a fixed bandwidth.

▶ We plot the asymptotic distribution of

$$\frac{\hat{f}_n(x) - E(\hat{f}_n(x))}{\sqrt{var(\hat{f}_n(x))}}$$

for x = 0 where we estimate  $E(\hat{f}_n(0))$  and  $var(\hat{f}_n(0))$  and put them and plot the histogram from the simulated data.

▶ We can clearly see that the histogram closely resembles that of a standard normal density as expected.



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• Since, for large n,

$$Z_{n}(x) = \frac{\widehat{f}_{n}(x) - E\widehat{f}_{n}(x)}{\sqrt{V\widehat{f}_{n}(x)}} \xrightarrow{\mathcal{L}} N(0,1)$$

where if we choose  $K(u) = \phi(u)$ , we get a closed form expression for the expectation term as,

$$\begin{split} E\widehat{f_n}\left(x\right) &= \int_{-\infty}^{\infty} \frac{1}{h_n} K_n\left(\frac{x-u}{h_n}\right) f\left(u\right) du \\ &= \frac{1}{2\pi h_n} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\left(\frac{x-u}{h_n}\right)^2} e^{-\frac{1}{2}u^2} du = (K_n \star f)\left(x\right) \\ &= \frac{1}{\sqrt{2\pi}\sqrt{h_n^2 + 1}} e^{-\frac{1}{2}\frac{x^2}{h_n^2 + 1}} = \frac{1}{\sqrt{h_n^2 + 1}} \phi\left(\frac{x}{\sqrt{h_n^2 + 1}}\right) \end{split}$$

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▶ and,

$$\sigma_n^2(x) = \frac{1}{n^2} \sum_{i=1}^n \operatorname{Var}\left(\frac{1}{h_n} K\left(\frac{x - X_i}{h_n}\right)\right)$$
$$\approx \frac{f(x)}{nh_n} \int_{-\infty}^{\infty} K^2(u) \, du$$
$$= \frac{f(x)}{nh_n} \frac{1}{2\sqrt{\pi}}$$

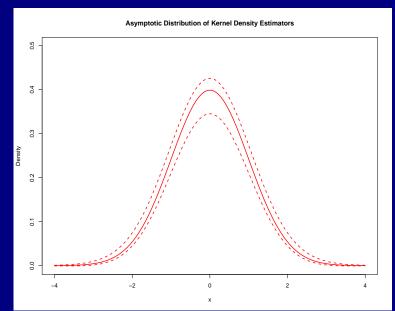
• While doing simulation, here we know the actual pdf f(x), hence we can use this property to visualize the CLT property of kernel density estimates by drawing upper and lower  $\alpha$  points for each of the values of x that gives us two nice curves like :-

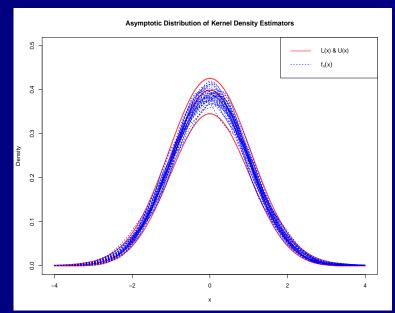
$$P\left(L_{\alpha}\left(x\right) \leq \widehat{f}_{n}\left(x\right) \leq U_{\alpha}\left(x\right)\right) \approx 1 - \alpha$$

▶ where ,

$$L_{\alpha}(x) = E\widehat{f}_{n}(x) - \tau_{\alpha/2}\sigma_{n}(x)$$
$$U_{\alpha}(x) = E\widehat{f}_{n}(x) + \tau_{\alpha/2}\sigma_{n}(x)$$

• if we draw these lines around the true density of the sample  $(\phi(x))$ , we get something like this :-





#### References

- Density Estimation for Statistics and Data Analysis by BW Silverman
- ▶ Nonparametric Functional Estimation by B.L.S Prakasa Rao
- ▶ All of Nonparametric Statistics by Larry Wasserman
- Elements of Statistical Learning by Trevor Hastie, Robert Tibshirani, Jerome H Friedman
- ▶ Another helpful read in this genre
- ▶ The Wikipedia page for KDE

#### Softwares and Tools used

- ▶ Google Colab R version for coding
- ▶ Overleaf online LaTeX editor
- ▶ Both are great for collaborative works/group projects.

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### THANK YOU

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